

# A classical Over Barrier Model to compute charge exchange between ions and one-optical-electron atoms

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In this paper we study theoretically the process of electron capture between one-optical-electron atoms (e.g. hydrogenlike or alkali atoms) and ions at low-to-medium impact velocities ( $v/v_e \leq 1$ ) working on a modification of an already developed classical Over Barrier Model (OBM) [V. Ostrovsky, J. Phys. B: At. Mol. Opt. Phys. **28** 3901 (1995)], which allows to give a semianalytical formula for the cross sections. The model is discussed and then applied to a number of test cases including experimental data as well as data coming from other sophisticated numerical simulations. It is found that the accuracy of the model, with the suggested corrections and applied to quite different situations, is rather high.

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## I. INTRODUCTION

The electron capture process in collisions of slow, highly charged ions with neutral atoms and molecules is of great importance not only in basic atomic physics but also in applied fields such as fusion plasmas and astrophysics. The process under study can be written as:

$$A^{+q} + B \rightarrow A^{(q-j)+} + B^{j+} \quad . \quad (1)$$

Theoretical models are regularly developed and/or improved to solve (1) from first principles for a variety of choices of target  $A$  and the projectile  $B$ , and their predictions are compared with the results of ever more refined experiments.

In principle, one could compute all the quantities of interest by writing the time-dependent Schrödinger equation for the system (1) and programming a computer to solve it. This task can be performed on present-days supercomputers for moderately complicated systems. Notwithstanding this, simple approximate models are still valuable: (i) they allow to get analytical estimates which are easy to adapt to particular cases; (ii) allow to get physical insight on the features of the problem by looking at the analytical formulas; (iii) finally, they can be the only tools available when the complexity of the problem overcomes the capabilities of the computers. For this reason new models are being still developed [1–3].

The present author has presented in a recent paper [3] a study attempting to develop a more accurate OBM by adding some quantal features. The model so developed was therefore called a semi-classical OBM. Its results showed somewhat an improvement with respect to other OBMs, but not a dramatic one.

In this paper we aim to present an OBM for dealing with one of the simplest processes (1): that between an ion and a target provided with a single active electron. Unlike the former one [3], this model is entirely developed within the framework of a classical model, previously studied in [1] (see also [4]), but with some important amendments and improvements which, as we shall see, allow a quite good accordance with experiments.

The paper is organized as follows: a first version of the model is presented and discussed in section II. In section III we will test our model against a first test case. From the comparison a further improvement to the model is proposed (section IV) and tested against the same case, as well as other data in section V. It will be shown that predictions with this correction are in much better agreement.

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## II. THE MODEL: FIRST PICTURE

We consider the standard scattering experiment and label  $\mathbf{T}$ ,  $\mathbf{P}$ , and  $\mathbf{e}$  respectively the target ion, the projectile and the electron. The system  $\mathbf{T} + \mathbf{e}$  is the initial neutral atom. Let  $\mathbf{r}$  be the electron vector relative to  $\mathbf{T}$  and  $\mathbf{R}$  the internuclear vector between  $\mathbf{T}$  and  $\mathbf{P}$ . In the spirit of classical OBM models, all particles are considered as classical objects.

Let us consider the plane  $\mathcal{P}$  containing all the three particles and use cylindrical polar coordinates  $(\rho, z, \phi)$  to describe the position of the electron within this plane. We can arbitrarily choose to set the angle  $\phi = 0$ , and assign the  $z$  axis to the direction along the internuclear axis.

The total energy of the electron is (atomic units will be used unless otherwise stated):

$$E = \frac{p^2}{2} + U = \frac{p^2}{2} - \frac{Z_t}{\sqrt{\rho^2 + z^2}} - \frac{Z_p}{\sqrt{\rho^2 + (R - z)^2}} \quad . \quad (2)$$

$Z_p$  and  $Z_t$  are the effective charge of the projectile and of the target seen by the electron, respectively. Notice that we are considering hydrogenlike approximations for both the target and the projectile. We assign an effective charge  $Z_t = 1$  to the target and an effective quantum number  $n$  to label the binding energy of the electron:  $E_n = Z_t^2/2n^2 = 1/2n^2$ .

As long as the electron is bound to  $\mathbf{T}$ , we can also approximate  $E$  as

$$E(R) = -E_n - \frac{Z_p}{R} \quad . \quad (3)$$

This expression is used throughout all calculations in (I); however, we notice that it is asymptotically correct as long as  $R \rightarrow \infty$ . In the limit of small  $R$ , instead,  $E(R)$  must converge to a finite limit:

$$E(R) \rightarrow (Z_p + 1)^2 E_n \quad (4)$$

(united atom limit). For the moment we will assume that  $R$  is sufficiently large so that eq. (3) holds, but later we will consider the limit (4), too.

On the plane  $\mathcal{P}$  we can draw a section of the equipotential surface

$$U(z, \rho, R) = -E_n - \frac{Z_p}{R} \quad . \quad (5)$$

This represents the limit of the region classically allowed to the electron. When  $R \rightarrow \infty$  this region is divided into two disconnected circles centered around each of the two nuclei. Initial conditions determine which of the two regions actually the electron lives in. As  $R$  diminishes there can be eventually an instant where the two regions become connected. In fig. 1 we give an example for this.

In the spirit of OBMs it is the opening of the equipotential curve between  $\mathbf{P}$  and  $\mathbf{T}$  which leads to a leakage of electrons from one nucleus to another, and therefore to charge exchange. We make here the no-return hypothesis: once crossed the barrier, the electron does not return to the target. It is well justified if  $Z_p \gg 1$ . As we shall see just below, this hypothesis has important consequences.

It is easy to solve eq. (5) for  $R$  by imposing a vanishing width of the opening ( $\rho_m = 0$ ); furthermore, by imposing also that there be an unique solution for  $z$  in the range  $0 < z < R$ :

$$R_m = \frac{(1 + \sqrt{Z_p})^2 - Z_p}{E_n} \quad . \quad (6)$$

In the region of the opening the potential  $U$  has a saddle structure: along the internuclear axis it has a maximum at

$$z = z_0 = R \frac{1}{\sqrt{Z_p} + 1} \quad (7)$$

while this is a minimum along the orthogonal direction.

Charge exchange occurs provided the electron is able to cross this potential barrier. Let  $N_\Omega$  be the fraction of trajectories which lead to electron loss at the time  $t$ . It is clear from the discussion above that it must be function of the solid opening angle  $\Omega$ , whose projection on the plane is the  $\pm\theta_m$  angle. The exact expression for  $N_\Omega$  will be given below. Further, be  $W(t)$  the probability for the electron to be still bound to the target, always at time  $t$ . Its rate of change is given by

$$dW(t) = -N_\Omega dt \frac{2}{T_{em}} W(t) \quad , \quad (8)$$

with  $T_{em}$  the period of the electron motion along its orbit.

It is important to discuss the factor  $dt(2/T_{em})$  since it is an important difference with (I), where just half of this value was used. The meaning of this factor is to account for the fraction of electrons which, within the time interval  $[t, t + dt]$  reach and cross the potential saddle. In (I) it was guessed that it should be equal to  $dt/T_{em}$ , on the basis of an uniform distribution of the classical phases of the electrons. However, let us read again what the rhs of eq. (8) does mean: it says that the probability of loss is given by the total number of *available* electrons within the loss cone ( $W(t) \times N_\Omega$ ), multiplied by the fraction of electrons which reach the potential saddle. However, on the basis of the no-return hypothesis, only outgoing electrons can contribute to this term: an electron which is within the loss cone and is returning to the target from the projectile is not allowed, it should already have been captured and therefore would not be in the set  $W$ . It is clear, therefore, that the effective period is  $T_{em}/2$ , corresponding to the outgoing part of the trajectory.

A simple integration yields the leakage probability

$$\begin{aligned} P_l &= P(+\infty) = 1 - W(+\infty) = \\ &= 1 - \exp\left(-\frac{2}{T_{em}} \int_{-t_m}^{+t_m} N_\Omega dt\right) . \end{aligned} \quad (9)$$

In order to actually integrate Eq. (9) we need to know the collision trajectory; an unperturbed straight line with  $b$  impact parameter is assumed:

$$R = \sqrt{b^2 + (vt)^2} . \quad (10)$$

The extrema  $\pm t_m$  in the integral (9) are the maximal values of  $t$  at which charge exchange can occur. If we identify this instant with the birth of the opening, using eq. (6) and (10), we find

$$t_m = \frac{\sqrt{R_m^2 - b^2}}{v} . \quad (11)$$

At this point it is necessary to give an explicit expression for  $N_\Omega$ . To this end, we will consider first the case of an electron with zero angular momentum ( $l = 0$ ), and then will extend to nonzero values.

In absence of the projectile, the classical electron trajectories, with zero angular momentum, are ellipses squeezed onto the target nucleus. We are thus considering an electron moving essentially in one dimension. Its hamiltonian can be written as

$$\frac{p^2}{2} - \frac{1}{r} = -E_n . \quad (12)$$

The electron has a turning point at

$$r_c = \frac{1}{E_n} . \quad (13)$$

Obviously the approaching of the projectile modifies these trajectories. However, in order to make computations feasible, we make the following hypothesis: electron trajectories are considered as essentially unperturbed in the region between the target and the saddle point. The only trajectories which are thus allowed to escape are those whose aphelia are directed towards the opening within the solid angle whose projection on the  $\mathcal{P}$  plane is  $\pm\theta_m$  (see fig. 1) *provided that* the turning point of the electron is greater than the saddle-point distance:  $r_c \geq z_0$ . The validity of these approximations can be questionable, particularly if we are studying the collision with highly-charged ions, which could deeply affect the electron trajectory. We limit to observe that it is necessary in order to make analytical calculations. *A posteriori*, we shall check the amount of error introduced by such an approximation.

The angular integration is now easily done, supposing a uniform distribution for the directions of the electrons:

$$N_\Omega = \frac{1}{2}(1 - \cos\theta_m) . \quad (14)$$

In order to give an expression for  $\theta_m$  we notice that  $\cos\theta_m = z_0/(\rho_m^2 + z_0^2)^{1/2}$ , with  $\rho_m$  root of

$$E(R) = \left(\rho_m^2 + \frac{R^2}{(\sqrt{Z_p} + 1)^2}\right)^{-1/2} + Z_p \left(\rho_m^2 + \frac{Z_p R^2}{(\sqrt{Z_p} + 1)^2}\right)^{-1/2} . \quad (15)$$

It is easy to recognize that, in the right-hand side, the first term is the potential due to the electron–target interaction, and the second is the electron–projectile contribution. Eq. (15) cannot be solved analytically for  $\rho_m$  except for the particular case  $Z_p = 1$ , for which case:

$$\rho_m^2 = \left( \frac{2}{E(R)} \right)^2 - \left( \frac{R}{2} \right)^2 . \quad (16)$$

The form of  $E(R)$  function of  $R$  cannot be given analytically, even though can be quite easily computed numerically [6]. In order to deal with expressions amenable to algebraic manipulations, we do therefore the approximation: first of all, divide the space in the two regions  $R < R_u, R > R_u$ , where  $R_u$  is the internuclear distance at which the energy given by eq. (3) becomes comparable with its united–atom form:

$$E_n + \frac{Z_p}{R_u} = (Z_p + 1)^2 E_n \rightarrow R_u = \frac{Z_p}{(Z_p + 1)^2 - 1} \frac{1}{E_n} . \quad (17)$$

We use then for  $E(R)$  the united–atom form for  $R < R_u$ , and the asymptotic form otherwise:

$$\begin{aligned} E(R) &= E_n + \frac{Z_p}{R}, & R > R_u \\ &= (Z_p + 1)^2 E_n, & R < R_u \end{aligned} \quad (18)$$

It is worthwhile explicitly rewriting eq. (16) for the two cases:

$$\begin{aligned} \rho_m^2 &= R^2 \left( \frac{4}{(E_n R + 1)^2} - \frac{1}{4} \right), & R > R_u \\ &= \frac{1}{4} \left( \frac{1}{E_n^2} - R^2 \right), & R < R_u \end{aligned} \quad (19)$$

and the corresponding expressions for  $N_\Omega$  are:

$$\begin{aligned} N_\Omega &= \frac{1 - \cos \theta_m}{2} = \frac{1}{8} (3 - E_n R), & R > R_u \\ &= \frac{1}{2} (1 - E_n R), & R < R_u . \end{aligned} \quad (20)$$

Note that  $N_\Omega = 1/2$  for  $R = 0$ . This is a check on the correctness of the model, since, for symmetrical scattering at low velocity and small distances we expect the electrons to be equally shared between the two nuclei.

When  $Z_p > 1$  we have to consider two distinct limits: when  $R \rightarrow \infty$  we know that eventually  $\rho_m \rightarrow 0$  (eq. 6). It is reasonable therefore to expand (15) in series of powers of  $\rho_m/R$  and, retaining only terms up to second order:

$$\rho_m^2 \approx \frac{2\sqrt{Z_p}}{(\sqrt{Z_p} + 1)^4} R^2 \left[ \left( \sqrt{Z_p} + 1 \right)^2 - Z_p - E_n R \right] . \quad (21)$$

Consistently with the limit  $R \rightarrow \infty$ , we have used the large- $R$  expression for  $E(R)$ .

The limit  $R \rightarrow 0$  is quite delicate to deal with: a straightforward solution of eq. (15) would give

$$\rho_m \approx \frac{1}{(Z_p + 1)E_n} + \mathcal{O}(R) , \quad (22)$$

but calculating  $\cos \theta_m$  and eventually  $N_\Omega$  from this expression gives wrong results: it is easy to work out the result  $N_\Omega = 1/2, R \rightarrow 0$ . This is wrong because, obviously, the limit  $N_\Omega \rightarrow 1, Z_p \rightarrow \infty$  must hold. The reason of the failure lies in the coupling of eq. (15) with the united–atom form for  $E(R)$ : one can notice that the expression thus written is perfectly symmetrical with respect to the interchange projectile–target. Because of this symmetry, electrons are forced to be equally shared between the two nuclei. This is good when dealing with symmetrical collisions,  $Z_p = Z_t = 1$ , and is actually an improvement with respect to (I), where eq. (21) was used even for small  $R$ ’s and one recovered the erroneous value  $N_\Omega(R=0) = 3/8$ . But when  $Z_p > 1$  the asymmetry must be retained in the equations. The only way we have to do this is to extend eq. (21) to small  $R$ , obtaining

$$1 - \cos \theta_m \approx \frac{\sqrt{Z_p}}{(\sqrt{Z_p} + 1)^2} \left[ \left( \sqrt{Z_p} + 1 \right)^2 - Z_p - E_n R \right] . \quad (23)$$

It is straightforward to evaluate eq. (23) in the limit  $Z_p \rightarrow \infty, R \rightarrow 0$ , and find the sought result, 2. We notice that, from the numerical point of view, it is not a great error using eq. (21) everywhere: the approximation it is based upon breaks down when  $R$  is of the order of  $R_u$  or lesser, which is quite a small range with respect to all other lengths involved when  $Z_p > 1$ , while even for the case  $Z_p = 1$  it is easy to recover (see equations below) that the relative error thus introduced on  $P_l$  is  $\Delta P_l/P_l = 1/24$  for small  $b$  (and—obviously—it is exactly null for large  $b$ ). Therefore, eq. (21) could be used safely in all situations. However, we think that the rigorous although quite lengthy derivation given above was needed since it is not satisfactory working with a model which does not comply with the very basic requirements required by the symmetries of the problem at hand.

We have now to take into account that the maximum excursion for the electron is finite. If we put  $r_c = z_0$  and use for  $z_0, r_c$  respectively the expressions given by (7) and (13), we obtain an equation which can be easily solved for  $R$ :

$$R = R'_m = (\sqrt{Z_p} + 1)r_c \quad . \quad (24)$$

The  $R'_m$  thus computed is the maximum internuclear distance at which charge exchange is allowed under the present assumptions. Since  $R'_m < R_m$  (compare the previous result with that of eq. 6) we have to reduce accordingly the limits in the integration in eq. (9): it must be performed between  $\pm t'_m$ , with the definition of  $t'_m$  the same as  $t_m$  but for the replacement  $R_m \rightarrow R'_m$ . The result for the leakage probability is:

$$P_l = 1 - \exp\left(-2\frac{F(u_m) + G_Z}{T_{em}}\right) \quad , \quad (25)$$

where we have defined

$$\begin{aligned} F(u) &= \frac{\sqrt{Z_p}}{(\sqrt{Z_p} + 1)^2} \left[ \left( (\sqrt{Z_p} + 1)^2 - Z_p \right) \frac{b}{v} u - \left( \frac{E_n b^2}{2v} \right) \left( u \sqrt{1 + u^2} + \operatorname{arcsinh}(u) \right) \right] \quad , \\ G_Z &= (3F(u_u) - 2t_u) \quad (Z_p = 1) \\ &= 0 \quad (Z_p > 1) \quad , \\ u_m &= vt'_m/b \quad , \\ u_u &= vt_u/b \quad , \\ t_u &= \frac{\sqrt{R_u^2 - b^2}}{v} \quad . \end{aligned} \quad (26)$$

The period can be easily computed by

$$T_{em} = 2 \int_0^{1/E_n} \frac{dr}{p} = \sqrt{2} \int_0^{1/E_n} \frac{dr}{\sqrt{\frac{1}{r} - E_n}} = 2\pi n^3 \quad (27)$$

(this result could be found also in [5]).

The cross section can be finally obtained after integrating over the impact parameter (this last integration must be done numerically):

$$\sigma = 2\pi \int_0^{b_m} b P_l(b) db \quad . \quad (28)$$

Again, we have used the fact that the range of interaction is finite: the maximum allowable impact parameter  $b_m$  is set equal to  $R'_m$ .

Finally, we consider the case when the angular momentum is different from zero. Now, orbits are ellipses whose minor semiaxis has finite length. We can still write the hamiltonian as function of just  $(r, p)$ :

$$\frac{p^2}{2} - \frac{1}{r} + \frac{L^2}{2r^2} = -E_n \quad . \quad (29)$$

$L$  is the usual term:  $L^2 = l(l+1)$ . The turning points are now

$$r_c^\pm = \frac{1 \pm \sqrt{1 - 2E_n L^2}}{2E_n} \quad . \quad (30)$$

and  $R'_m = (\sqrt{Z_p} + 1)r_c^+$ .

Now the fraction of trajectories entering the loss cone is much more difficult to estimate. In principle, it can still be determined: it is equal to the fraction of ellipses which have intersection with the opening. Actual computations can be rather cumbersome. Thus, we use the following approximation, which holds for low angular momenta  $l \ll n$  (with  $n$  principal quantum number): ellipses are approximated as straight lines (as for the  $l = 0$  case), but their turning point is correctly estimated using eq. (30). Note that also the period is modified: its correct expression is

$$T_{em} = \sqrt{2} \int_{r^-}^{r^+} \frac{dr}{\sqrt{\frac{1}{r} - E_n - \frac{l(l+1)}{2r^2}}} . \quad (31)$$

### III. A TEST CASE

As a first test case we consider the inelastic scattering  $\text{Na}^+ + \text{Na}(28d, 29s)$ . We investigate this system since: (i) it has been studied experimentally in [7]; (ii) some numerical simulations using the Classical Trajectory Monte Carlo (CTMC) method have also been done on it [8], allowing to have detailed informations about the capture probability  $P_l$  function of the impact parameter, and not simply integrated cross sections; (iii) finally, it has been used as test case in (I), thus allowing to assess the relative quality of the fits.

In fig. (2) we plot the normalized cross section  $\tilde{\sigma} = \sigma/n^4$  versus the normalized impact velocity  $\tilde{v} = vn$  for both collisions  $nl = 28d$  and  $nl = 29s$  (solid line). The two curves are very close to each other, reflecting the fact that the two orbits have very similar properties: the energies of the two states differ by a very small amount, and in both cases  $E_n L^2 \ll 1$ . The two curves show reversed with respect to experiment:  $\sigma(28d)$  it is greater than  $\sigma(29s)$ . The reason is that the parameter  $r_c$  is larger in the former case than in the latter.

We can distinguish three regions: the first is at reduced velocity around 0.2, where a steep increase of cross section appears while going towards lower velocities. Over-barrier models do not appear to fully account for this trend: they have a behaviour at low speed which is ruled approximately by the  $1/v$  law, consequence of the straight-line impact trajectory approximation: it is well possible that this approximation too becomes unadequate in this region.

The second region covers roughly the range  $0.3 \div 1.0$ . Here the  $nl = 29s$  data are rather well simulated while the present model overestimates the data for  $nl = 28d$ . The bad agreement for  $nl = 28d$  was already clear to Ostrovsky which attributed it to a deficiency of the model to modelize  $l$ -changing processes. It seems clear that neither our treatment of the angular momentum is sufficient to cure this defect.

Finally, there is the region at  $\tilde{v} > 1$ , where again the OBM, as it stands, is not able to correctly reproduce the data. The reason for this discrepancy can be traced back to the finite velocity of the electron: the classical electron velocity is  $v_e = 1/n$ , so  $\tilde{v}$  can be given the meaning of the ratio between the projectile and the electron velocity. When  $\tilde{v} \geq 1$  the projectile is less effective at collecting electrons in its outgoing part of the trajectory (i.e. when it has gone beyond the point of closest approach). In simple terms: an electron is slower than the projectile; when it is left behind, it cannot any longer reach and cross the potential barrier.

### IV. CORRECTIONS TO THE MODEL

This picture suggests a straightforward remedy: a term must be inserted in eq. (8) to account for the diminished capture efficiency. This is accomplished formally through rewriting  $N_\Omega \rightarrow w(t, \tilde{v})N_\Omega$ , with  $w \leq 1$ . We have put into evidence that  $w$  can in principle be function of time and of the impact velocity. The simplest correction is made by assuming a perfect efficiency for  $\tilde{v} < 1$ ,  $w(t, \tilde{v} < 1) = 1$ , while, for  $\tilde{v} > 1$ , no electrons can be collected after that the distance of minimum approach has been reached:  $w^+ \equiv w(t > 0, \tilde{v} > 1) = 0$ . This can appear too strong an assumption, since those electrons which are by the same side of the projectile with respect to the nucleus, and which are close to their turning point may still be captured. In fig. (2) we can compare the original data with those for  $w^+ = 0$  (dashed line). The sharp variation of  $\sigma$  at  $\tilde{v} = 1$  is obviously a consequence of the crude approximations done choosing  $w$  which has a step-like behaviour with  $v$ .

To get further insight, we plot in fig. 3 the quantity  $bP_l(b)$  versus  $b$  for the collision  $\text{Na}^+ + \text{Na}(28d)$ . The impact velocity is  $\tilde{v} = 1$ . The symbols are the CTMC results of ref. [8]. Solid line is the model

result for  $w^+ = 1$ ; dotted line, the result for  $w^+ = 0$ ; dashed line, an intermediate situation, with  $w^+ = 1/2$ . Striking features are, for all curves, the nearly perfect accordance of the value  $b \approx 3000$  at which  $P_l = 0$  (it is  $b_m$  according to our definition). The behaviour at small  $b$ 's ( $P_l \approx 1/2$ ) is well reproduced for  $w^+ = 1$  while it is slightly underestimated by the two other curves. On the other hands, only by setting  $w^+ = 0$  it is possible to avoid the gross overestimate of  $P_l$  near its maximum.

It is thus evident that the agreement is somewhat improved in the region  $\tilde{v} \approx 1$  by letting  $w^+ = 0$ . However, the high-velocity behaviour is still missed by the model, which predicts a power-law behaviour  $\sigma \propto v^{-1}$ , while the actual exponent is higher. Within our picture, this suggests that also the capture efficiency  $w^- = w(t < 0)$  must be a decreasing function of  $\tilde{v}$ . An accurate modelization of the processes which affect this term is difficult, and we were not able to provide it. However, some semi-qualitative arguments can be given. Let us review again the process of capture as described in section II and shown in fig. (1): if  $\tilde{v} > 1$ , an electron at time  $t$  can be in the loss cone and still not to be lost, since within a time span  $\Delta t \approx \rho_m/v$  the position of the loss cone has shifted of such an amount that only those electrons which were closer to the saddle point than a distance  $v_e \Delta t$  could be caught. The fraction of these electrons is  $\Delta t(2/T_{em}) \approx \rho_m(2/vT_{em})$ . This correction gives an additional  $1/v$  dependence, thus now  $\sigma \approx 1/v^2$ .

As an exercise, we try to fit experimental data using  $w$  as a free parameter instead that a function to be determined by first principles. We choose one of the simplest functional forms:

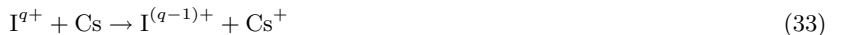
$$w = \frac{1 + |\beta|^m}{1 + |\tilde{v} - \beta|^m} \quad , \quad (32)$$

with  $\beta, m$  free parameters to be adjusted. This form gives the two correct limits:  $w \rightarrow 1, \tilde{v} \rightarrow 0$ , and  $w \rightarrow 0, \tilde{v} \rightarrow \infty$ . The parameter  $\beta$  is not really needed; it has been added to reach a better fit. Its meaning is that of a threshold velocity, at which the capture efficiency begins to diminish. In fig. (2) we plot the fit obtained with  $\beta = 0.2, m = 4$  (dotted line): this is not meant to be the best fit, just a choice of parameters which gives a very good agreement with data. We see that the suggested corrections are still not enough to give the right power-law, if one needs to go to some extent beyond the region  $\tilde{v} = 1$ .

## V. OTHER COMPARISONS

### A. Iodine - Cesium collisions

We apply now our model to the process of electron capture



with  $q = 6 \div 30$ . This scattering process has been studied experimentally in [9]. It is particularly interesting to study in this context since it has revealed untractable by a number of other OBM's, including that of (I) (for a discussion and results, see [3]). The impact energy is chosen equal to  $1.5 \times Z_p$  keV: since it corresponds to  $\tilde{v} \ll 1$ , we can safely assume  $w = 1$ . The Cesium atom is in its ground state with the optical electron in a  $s$  state.

In fig. 4 we plot the experimental points together with our estimates. In this case the fit is excellent. It is important to notice that this agreement is entirely consequence of our choice of limiting integration to  $R$  given by eq. (24): to understand this point, observe that because of the very high charge of the projectile, the exponential term in eq. (25) is small ( $F$ , by direct inspection, is increasing with  $Z_p$ ) and thus  $P_l \approx 1$ . The details of the model which are in  $F$  are therefore of no relevance. The only surviving parameter, and that which determines  $\sigma$ , is  $R'_m$ . It can be checked by directly comparing our fig. 4 with fig. 1 of ref. [3], where results from model (I) are shown, which differ from ours just in replacing eq. (24) with eq. (6). There, the disagreement is severe.

### B. Ion - Na( $n = 3$ ) collisions

As a final test case we present the results for collisions H-Na(3s,3p). They are part of a set of experiments as well as numerical simulations involving also other singly-charged ions: He, Ne, and Ar (see [11] and the references therein and in particular [12]; ref. [13] presents numerical calculations for the same system). In fig. 5 we plot the results of our model together with those of ref. [11]. Again, we find that only by neglecting  $w^+$  some accordance is found. The low-energy wing of the

curve is strongly underestimated for Na(3s), while the agreement is somewhat better for Na(3p). Again, the slope of  $\sigma$  for relative velocities higher than 1 could not be reproduced. We do not show results for other ions: they can be found in fig. 3 of ref. [11]. What is important to note is that differences of a factor two (and even larger for 3s states) appear between light ( $H^+$ ,  $He^+$ ) and heavy ( $Ne^+$ ,  $Ar^+$ ) ions which our model is unable to predict. We can reasonably conclude therefore: (i) that the present model is not satisfactory for  $v/v_e < 1$  (it was already pointed out in sec. IV) and for  $v/v_e > 1$ ; (ii) the structure of the projectile must be incorporated into the model otherwise different ions with the same charge should cause the same effect, at odds with experiments. As emphasized in [11,12] the energy defect  $\Delta E$  of the process is a crucial parameter: captures to states with  $\Delta E \approx 0$  are strongly preferred. Obviously, the value of  $\Delta E$  depends on the energy levels structure of the recombining ion.

## VI. SUMMARY AND CONCLUSIONS

We have developed in this paper a classical OBM for single charge exchange between ions and atoms. The accuracy of the model has been tested against three cases, with results going from moderate-to-good (sec. III and IV), excellent (sec. V.A), and poor-to-moderate (sec. V.B). As a rule of thumb, the model can be stated to be very well suited for collisions involving highly charged ions at low velocities.

The model is based upon a previous work [1], and adds to it a number of features, which we go to recall and discuss: (i) the finite excursion from the nucleus permitted to the electrons; (ii) the redefinition of the fraction of lost electrons  $dt/T_{em} \rightarrow dt(2/T_{em})$ ; (iii) a more accurate treatment of the small impact parameter region for symmetrical collisions; (iv) the explicit-although still somewhat approximate-treatment of the capture from  $l > 0$  states; (v) a correction to the capture probability due finite impact velocity. Let us discuss briefly each of these points:

Point (i) and (ii) contribute a major correction: in particular, (i) is essential to recover that excellent agreement found in section V.A, while (ii) accounts for the correct  $bP_l$  behaviour at small  $b$ 's (see fig. 2).

Point (iii) is unimportant for actual computations, but corrects an inconsistency of the model.

Point (iv) has been studied in less detail, in part for the lack of experimental data on which doing comparisons.

Point (v): a good theoretical estimate of  $w$  should be of the outmost importance for developing a really accurate model of collision at medium-to-high impact velocity. In this paper we have just attempted a step towards this direction which, however, has allowed to recover definitely better results.

Finally we recall from sec. V.B that the treatment of the projectile-or better the process of the electron-projectile binding-is an aspect which probably awaits for main improvements. We just observe that it is a shortcoming of all classical methods, that they cannot easily deal with quantized energy levels.

## ACKNOWLEDGMENTS

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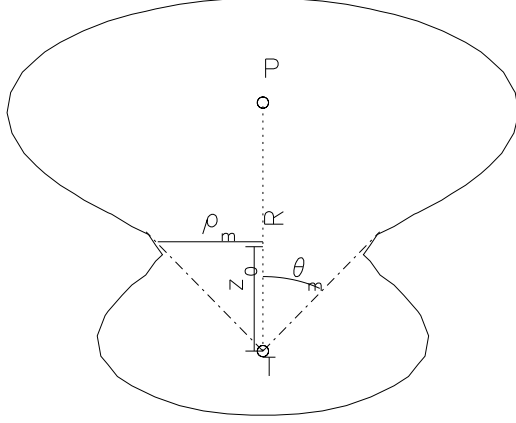


FIG. 1. The enveloping curve shows a section of the equipotential surface  $U = E$ , i.e. it is the border of the region classically accessible to the electron.  $R$  is the internuclear distance. The parameter  $\rho_m$  is the radius of the opening which joins the potential wells,  $\theta_m$  the opening angle from  $\mathbf{T}$ ;  $z_0$  is the position of the potential's saddle point.

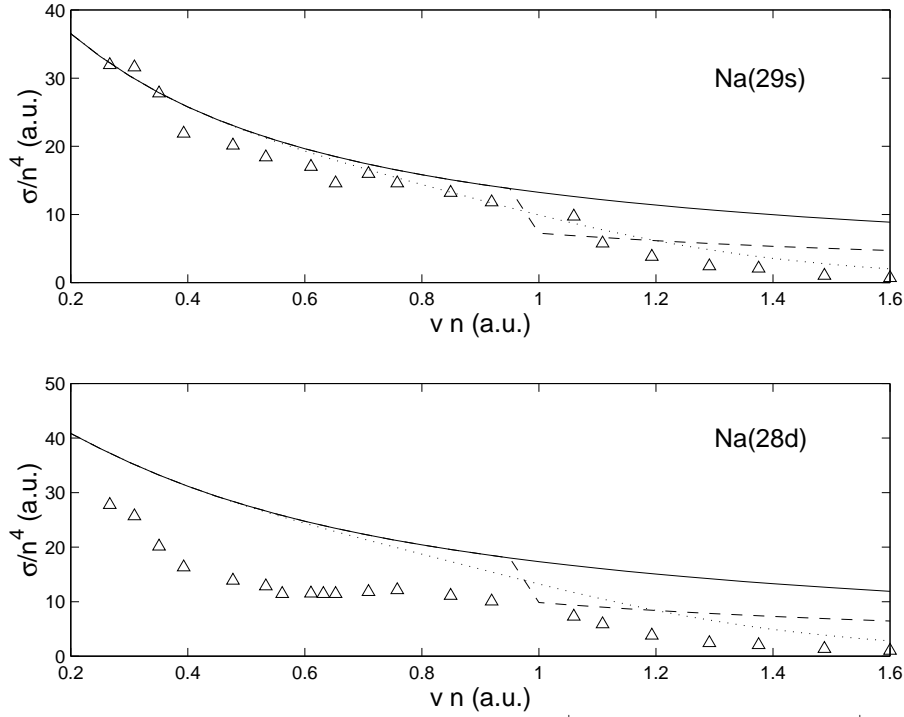


FIG. 2. Cross section for charge exchange for  $\text{Na}^+ - \text{Na}(29s)$  (upper) and  $\text{Na}^+ - \text{Na}(28d)$  (lower) collisions. Symbols, experimental data (adapted from ref. 7); solid line, present model with  $w^+ = 1$ ; dashed line, model with  $w^+ = 0$ ; dotted line, model with  $w$  given by eq. (32). Note that the experimental results are not absolutely calibrated, the data shown here are calibrated using as reference the CTMC results at  $\tilde{v} = 1$  and  $nl = 28d$ .

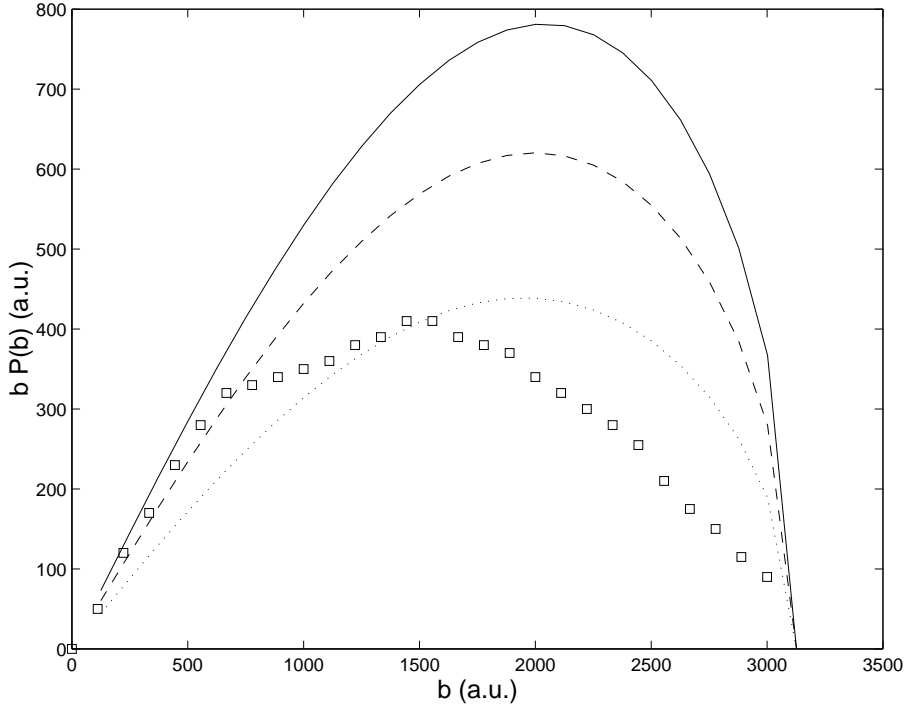


FIG. 3. Probability of electron capture multiplied by impact parameter,  $P_l b$ , for  $\text{Na}^+ - \text{Na}(28d)$  collision at  $\tilde{v} = 1$ . Squares, CTMC data (adapted from ref. 8); solid line, present model with  $w^+ = 1$ ; dashed line,  $w^+ = 0.5$ ; dotted line,  $w^+ = 0$ .

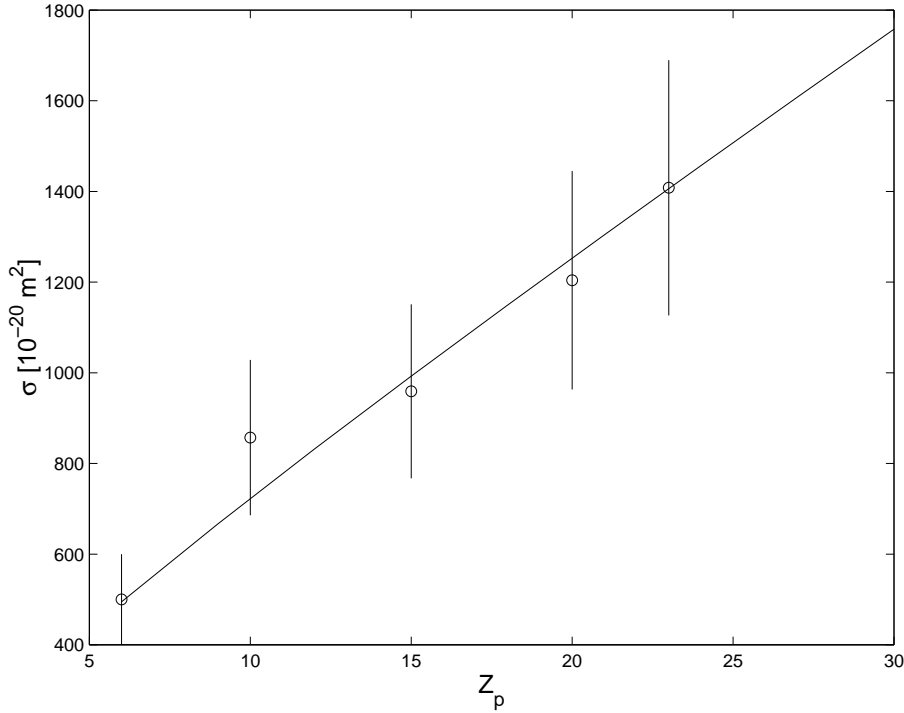


FIG. 4. Cross section for charge exchange in  $\text{I}^{+q} - \text{Cs}$  collisions. Circles, experimental data with 20% error bar; solid line, present model (where we have set  $w \equiv 1$ , since we are dealing with  $v/v_e \ll 1$ ).

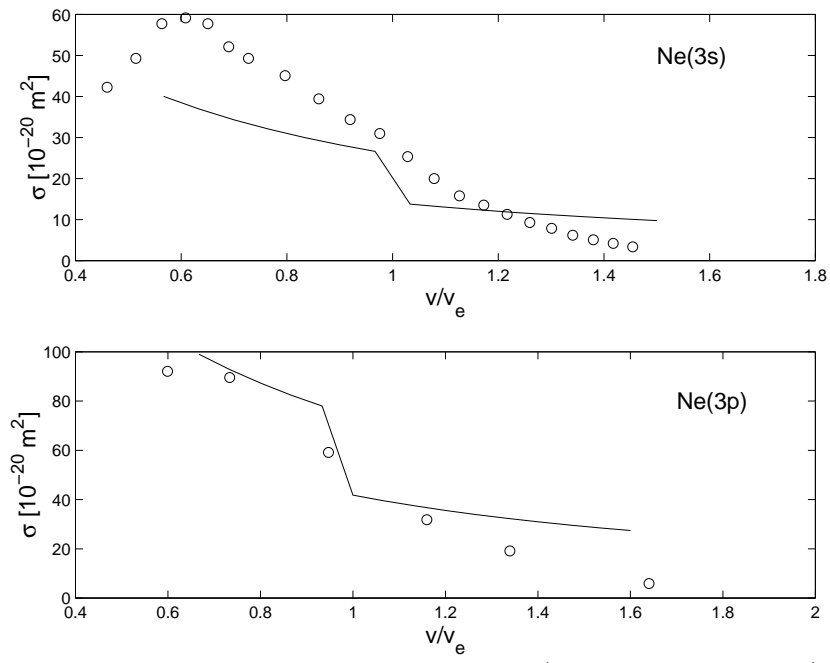


FIG. 5. Cross section for charge exchange in  $\text{H}^+ - \text{Na}(3s)$  (upper) and  $\text{H}^+ - \text{Na}(3p)$  (lower) collisions. Symbols, experimental data from ref. (9); lines, present model.